Isophthalic acid, monoamide, N-(2-fluorophenyl)-, heptyl ester

Inchi: InChI=1S/C21H24FNO3/c1-2-3-4-5-8-14-26-21(25)17-11-9-10-16(15-17)20(24)23-19-13-

InchiKey: HPFVLEHPYKDUIW-UHFFFAOYSA-N

Formula: C21H24FNO3

SMILES: CCCCCCCOC(=O)c1cccc(C(=O)Nc2ccccc2F)c1

Mol. weight [g/mol]: 357.42

Physical Properties

Property code	Value	Unit	Source
gf	-136.76	kJ/mol	Joback Method
hf	-526.67	kJ/mol	Joback Method
hfus	50.02	kJ/mol	Joback Method
hvap	89.74	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.205		Crippen Method
mcvol	279.990	ml/mol	McGowan Method
pc	1568.47	kPa	Joback Method
rinpol	2973.00		NIST Webbook
tb	922.80	K	Joback Method
tc	1143.43	K	Joback Method
tf	579.65	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.38	J/mol×K	922.80	Joback Method
cpg	886.76	J/mol×K	959.57	Joback Method
cpg	898.96	J/mol×K	996.34	Joback Method
cpg	910.03	J/mol×K	1033.12	Joback Method
cpg	920.03	J/mol×K	1069.89	Joback Method
cpg	929.02	J/mol×K	1106.66	Joback Method
cpg	937.04	J/mol×K	1143.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345781&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume